

Fuel Research at UTRC

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Multi-Agency Coordinating Council for Combustion Research
Sandia National Laboratories, Livermore, CA

September 17-20, 2012



**United Technologies
Research Center**



Background

- Secure supply
 - Military needs guaranteed fuel supply in time of war
- Global Warming:
 - Combustion of fossil-derived fuels
 - Combustion emissions (soots/particulates)
- Physics-based combustor models
 - Existing models barely sufficient for design predictions
- Physical vs. chemical effects
 - Typically, physical effects presumed to dominate (except soot)
- Complexity of fuels
 - Large number of species
 - Unknown/uncertain reaction rate laws
- DoD needs
 - AF – 50% utilization of alternative fuels by 2016 (in US)
 - Navy - Sailing the 'Great Green Fleet' by 2016/50% Utilization by 2020
 - SERDP – Understand impact on emissions

Acknowledgements

- Sharon Beermann-Curtin
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- Dale Shouse

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- Tony Dean
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- Bill Pitts
- Tom Litzinger
- Jeff Lovett
- Heidi Hollick



Objectives and Outline

Objectives:

- Develop/apply methods/tools that can incorporate both physical and chemical effects to predicting impact on engine performance

Outline:

- New data sets – performance of fuels in research combustor
 - Fuel selection
 - Combustor
 - Emissions, LBO data
 - Surrogates and Predictions
- Hydrocarbon Emission Fingerprint
 - Discussion of controlling phenomena
 - Quantitative comparisons
- Brief update/comments on AF Rules and Tools program
- Summary
- Recommendations

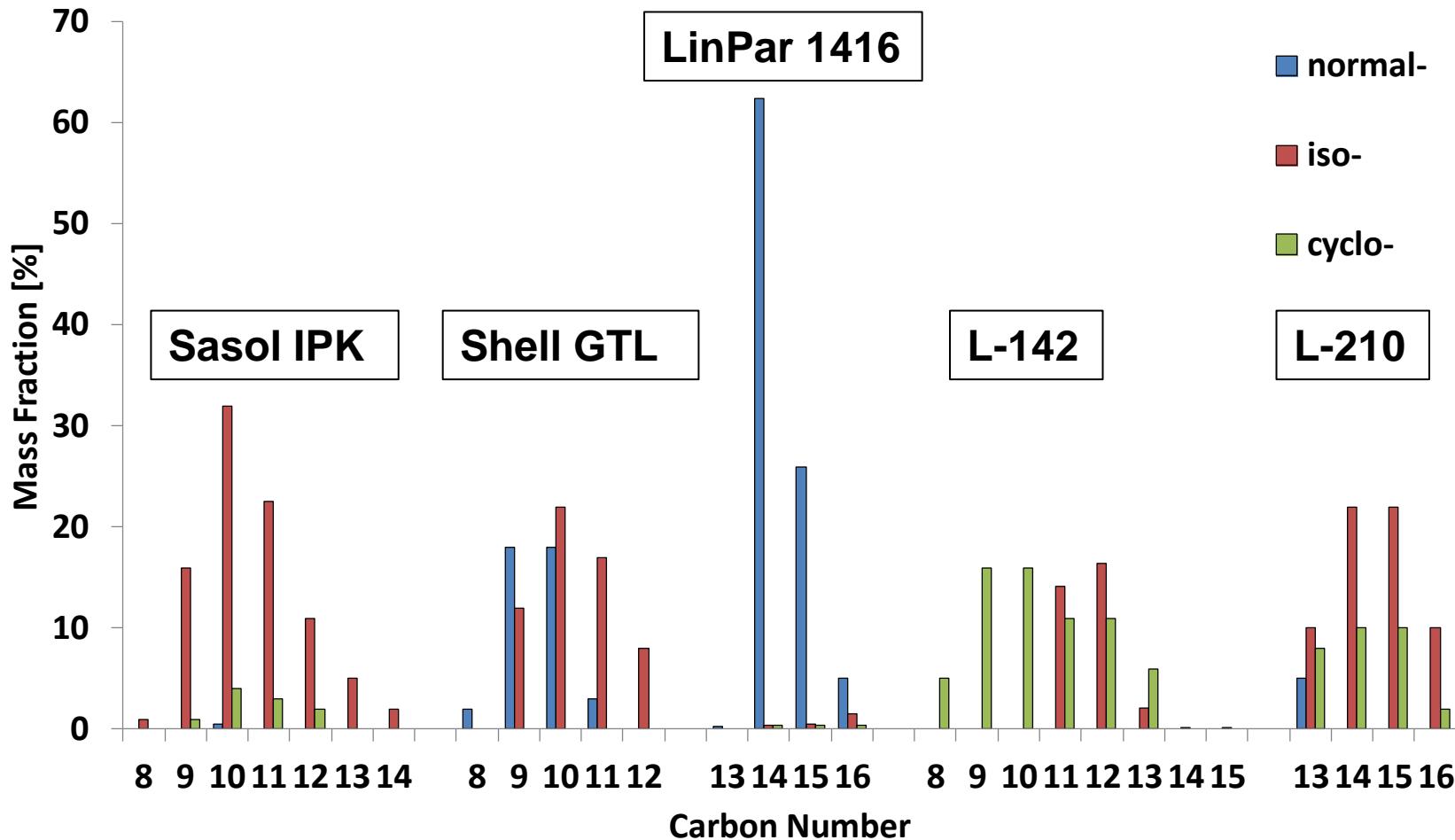
Combustor Validation Data – Fuels Tested

Feedback from ONR – We need combustor data for different fuels!

Fuels	Description	Mean MW	Flash Point [C]	Density [g/ml]	Boiling Pt. [C]		Cetane #
Jet-A	<i>Baseline</i>				IBP	FBP	
JP-5	<i>Baseline</i>		63	0.815	182	253	43.0
HRJ	ONR Supplied, Camelina based alternate fuel		62	0.768	174	286	66.0
JP-5							
Sasol IPK	Coal-derived kerosene, supplied by AFRL (POS 7629)	149	53	0.765	174	232	31.3
Shell GTL	Natural gas based gas-to-liquid kerosene, supplied by AFRL (POS 5729)	137	43	0.736	154	195	58.4
LinPar 1416	Low aromatic solvent	201	117	0.768	247	277	81.8*
L-142	Low aromatic solvent	156	61	0.804	177	233	46.5*
L-210	Low aromatic solvent	193	96	0.825	240	283	53.1*

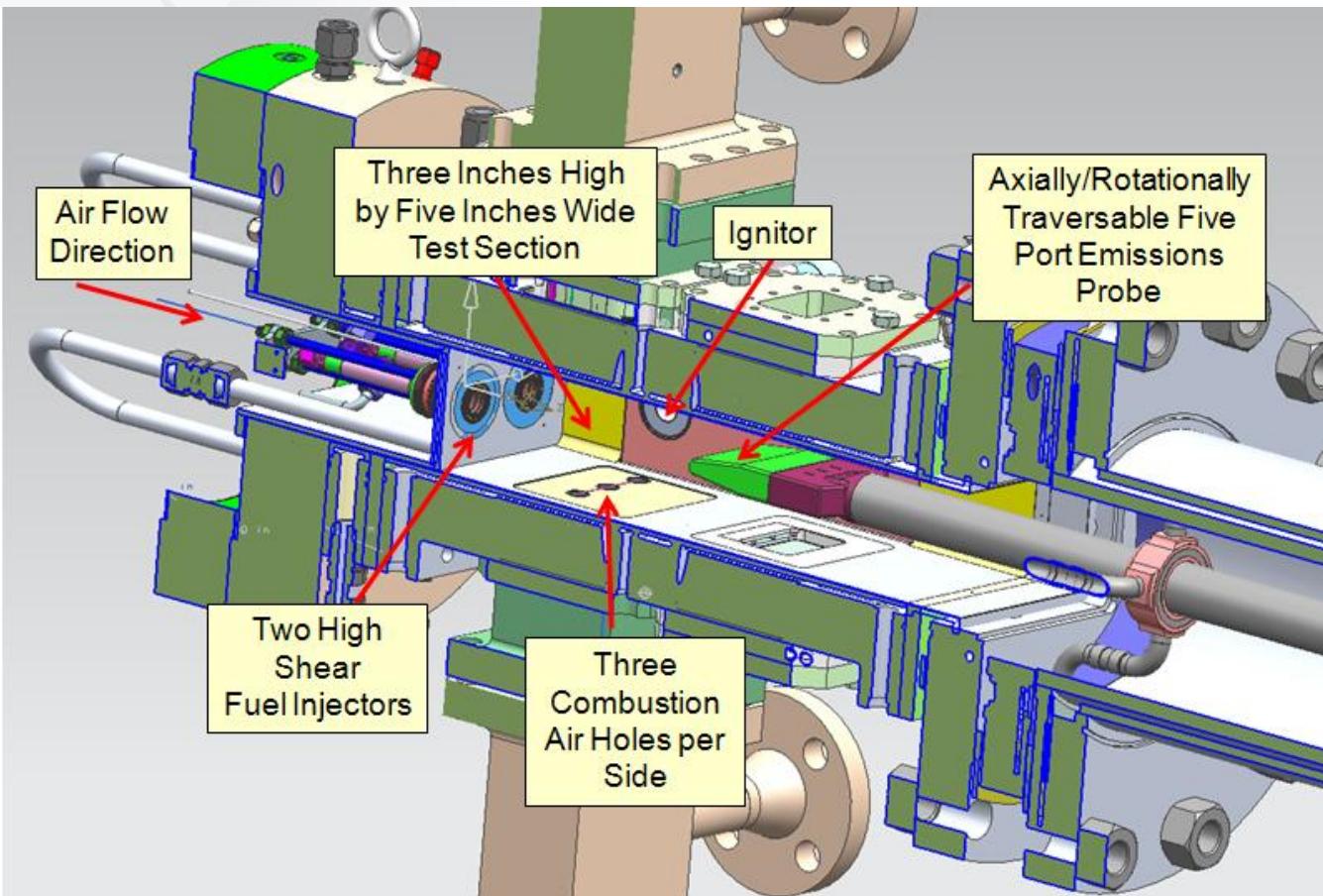
Combustor Validation Data – Fuels

Solvents and synthetic fuels explore contrasting physical/chemical changes



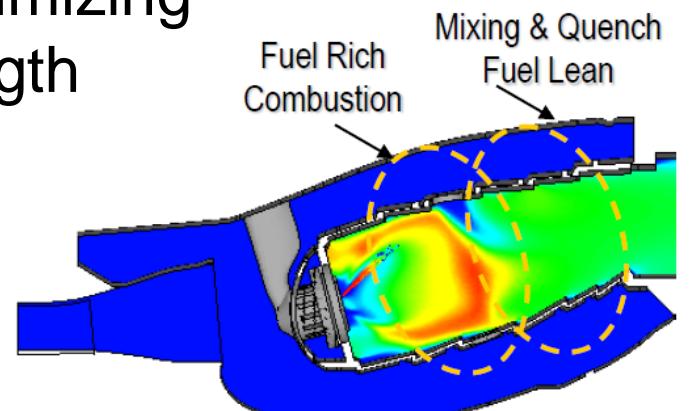
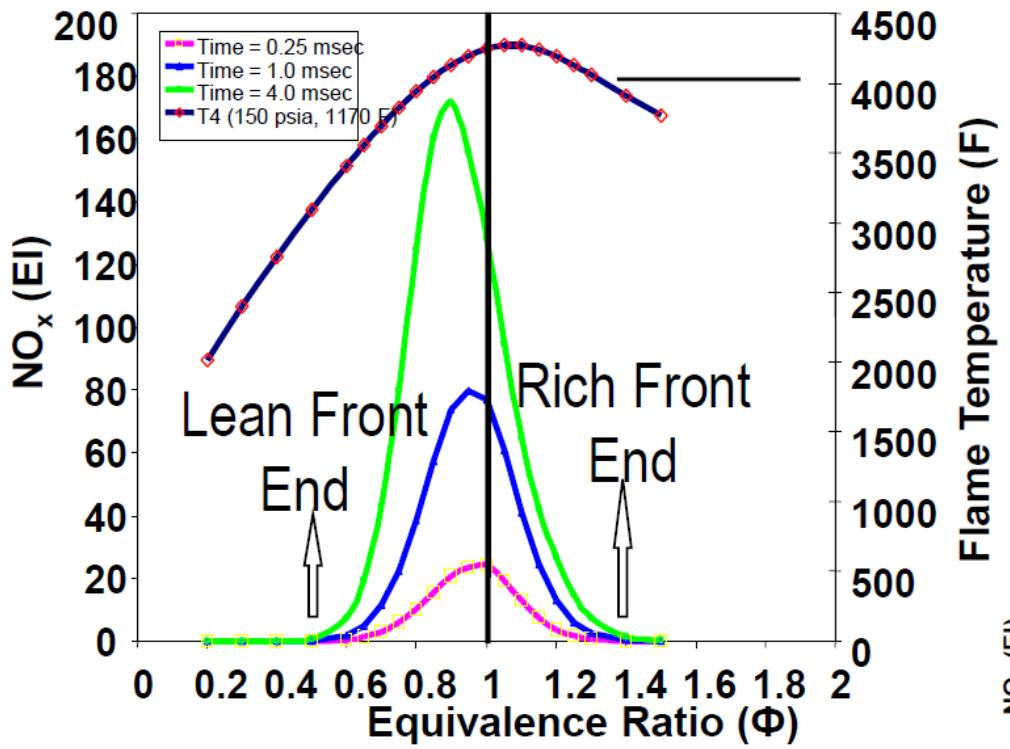
Combustor Validation

- Validation data sets for JP-5 and alternatives
 - Testing performed in UTRC JBTS facility
 - Rig simulates conventional combustor flowpath/operation

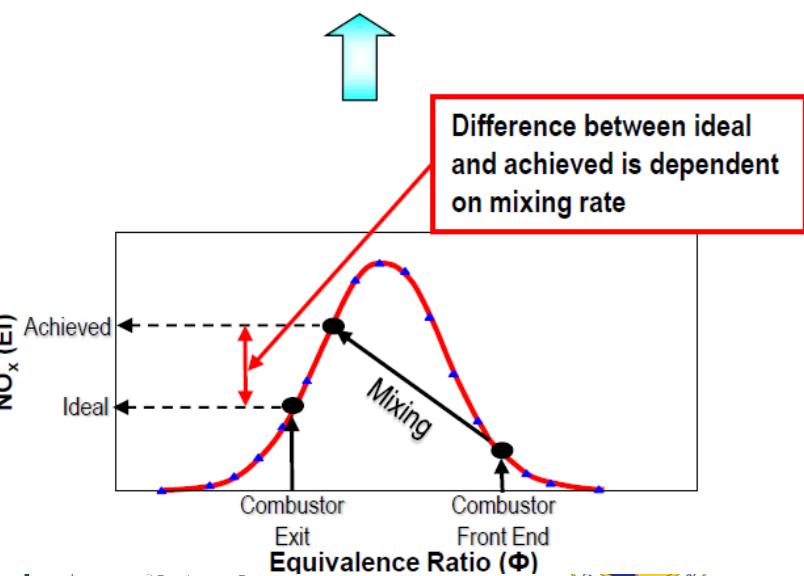


Rich-Quench-Lean (RQL) Combustor Technology

- Optimized for operability while minimizing NOx emissions and combustor length

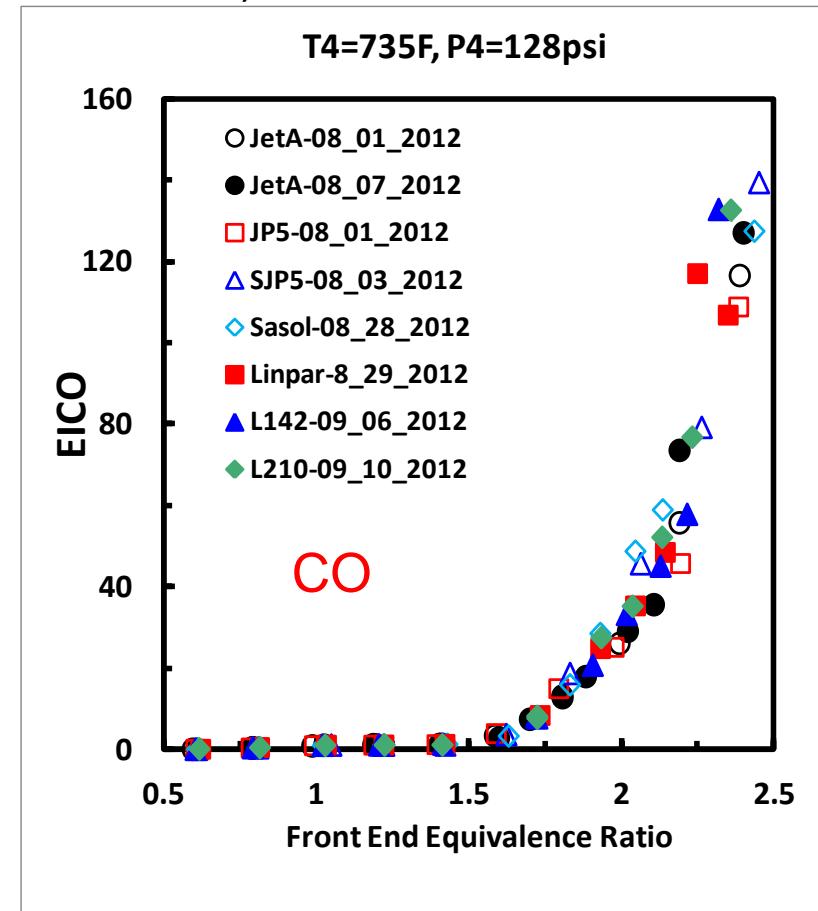
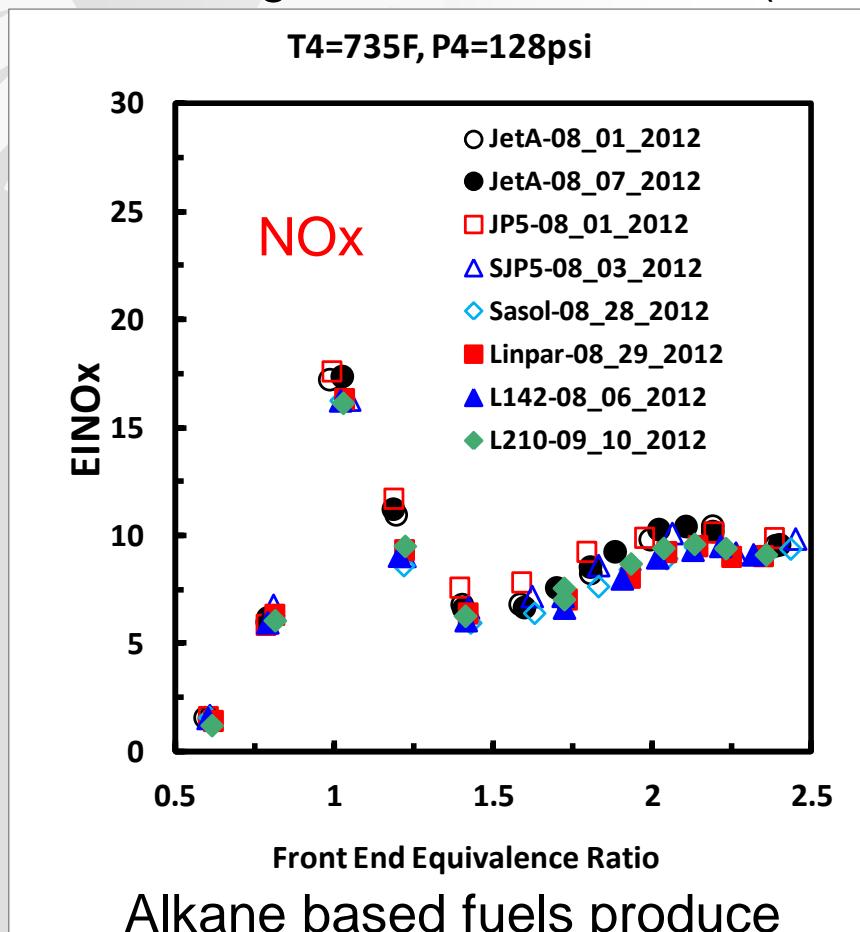


Rich Quick Quench Lean (RQL)



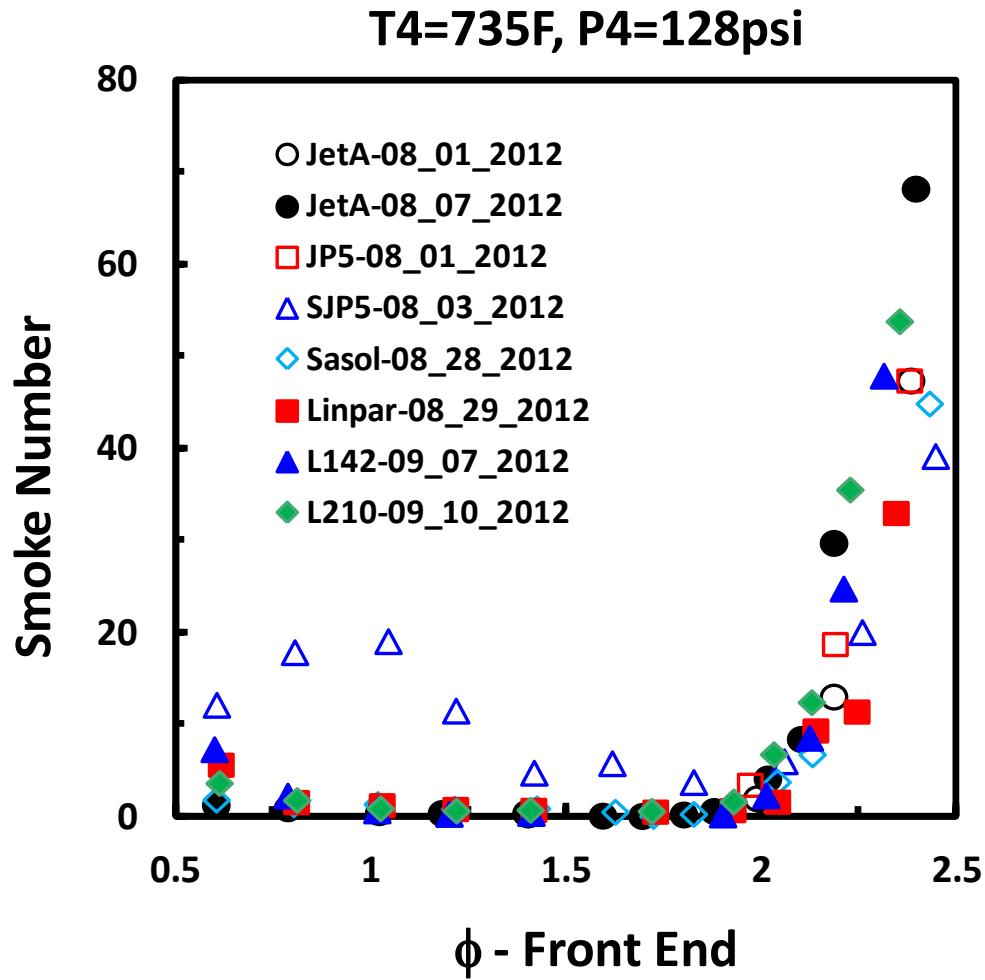
Combustor Validation Data – Emissions

- Small changes for NOx and CO (emission indexes)



Combustor Validation Data – Emissions

- Smoke data for several jet fuels and solvents



Alkane based fuels
(synthetic jet fuels and
solvents) produce less
soot.

Anomalous high soot
levels at low f/a ratios
for Camelina HRJ
(SJP5)

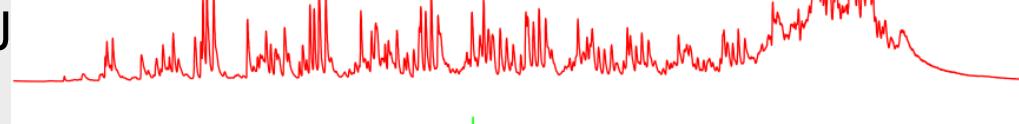
Fuels Analyzed (courtesy of Tonghun Lee (MSU))

Anomalous soot possibly due to large concentration of high MW species

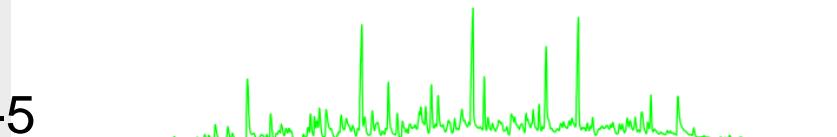
Camelina HRJ
(JP-8)



Camelina HRJ
(JP-5)



Petroleum JP-5



Retention Time [min]

- Navy & Air Force Fuels Total Ion Chromatograms

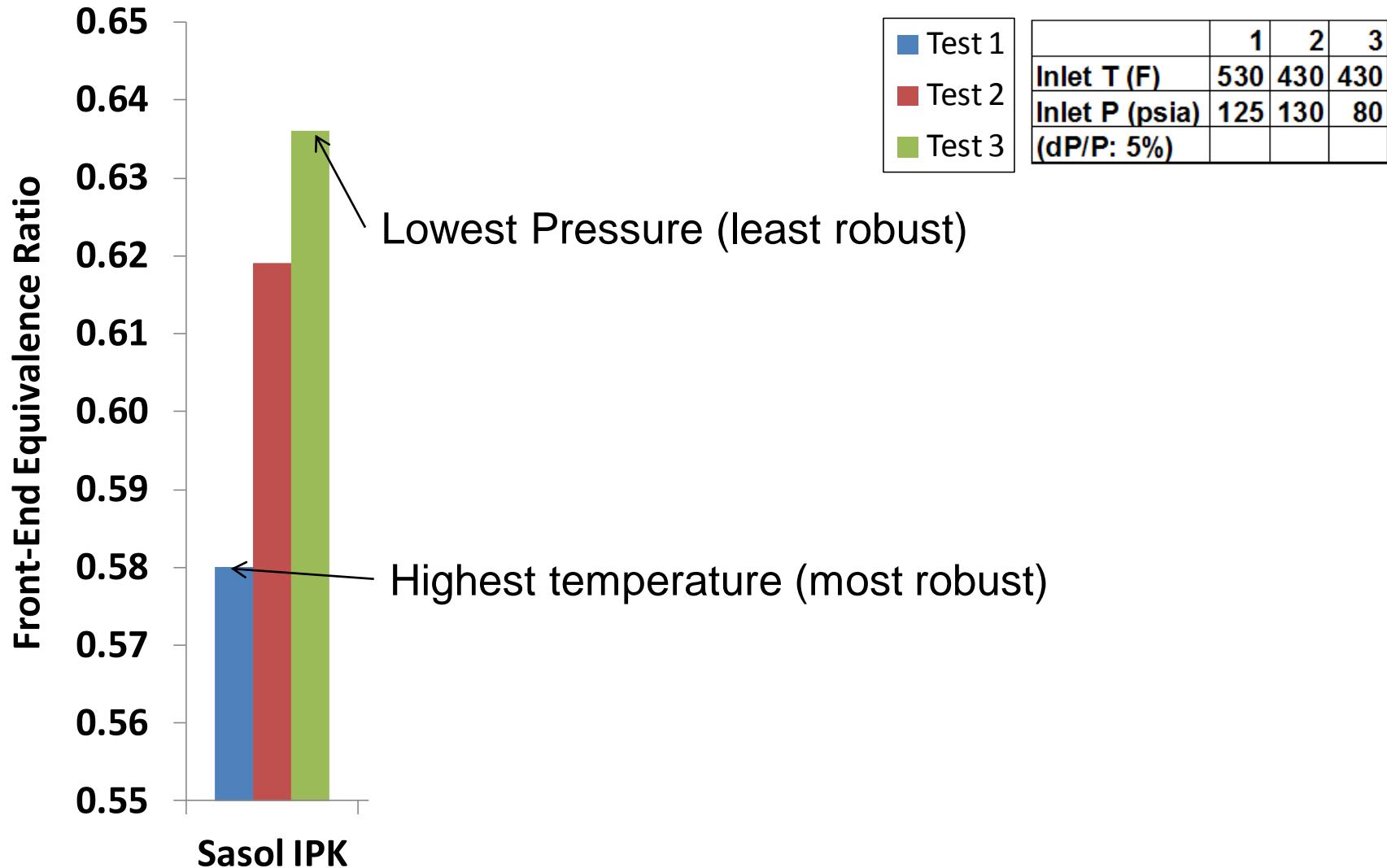


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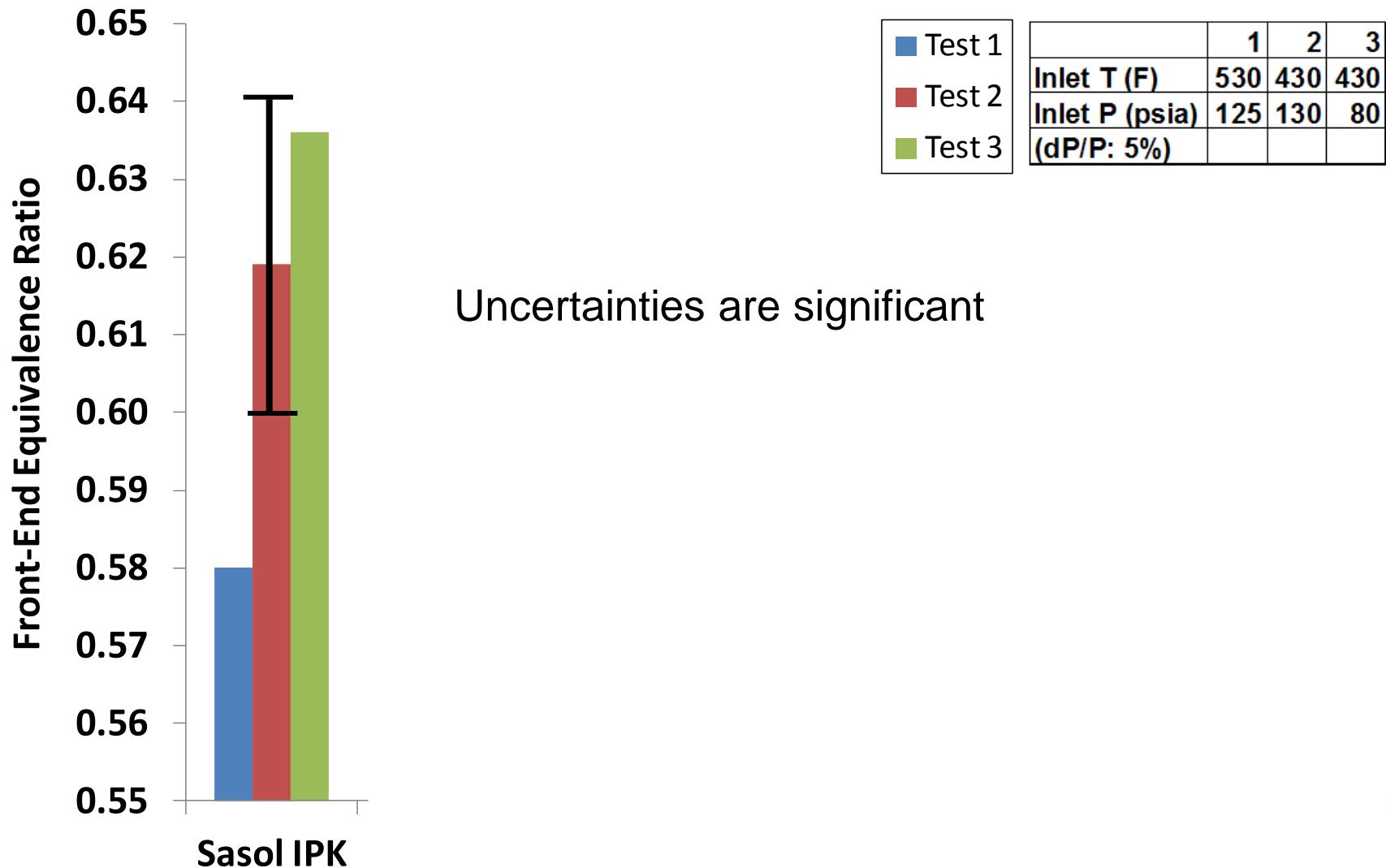
Combustor Validation Data – Lean Blow Off

- Lean Blow-Out (LBO) data



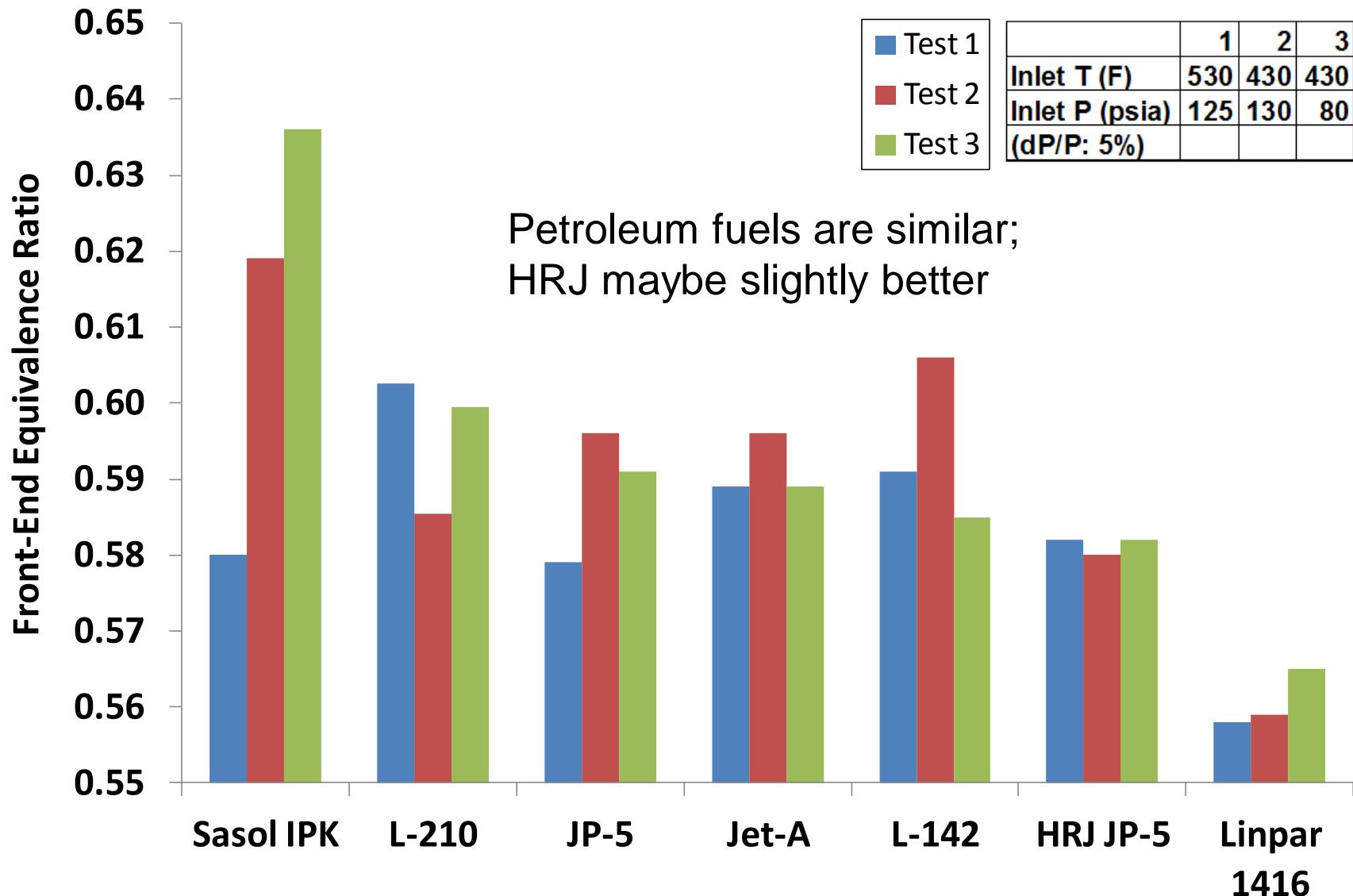
Combustor Validation Data – Lean Blow Off

- LBO data



Combustor Validation Data – Lean Blow Off

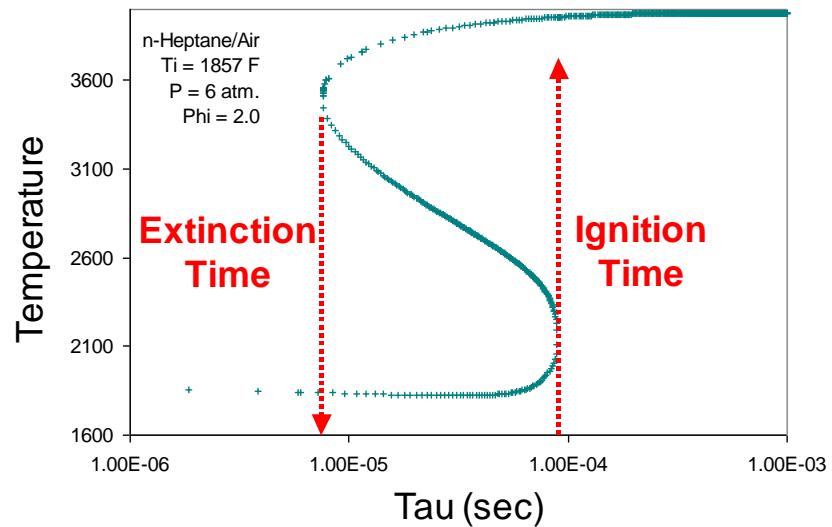
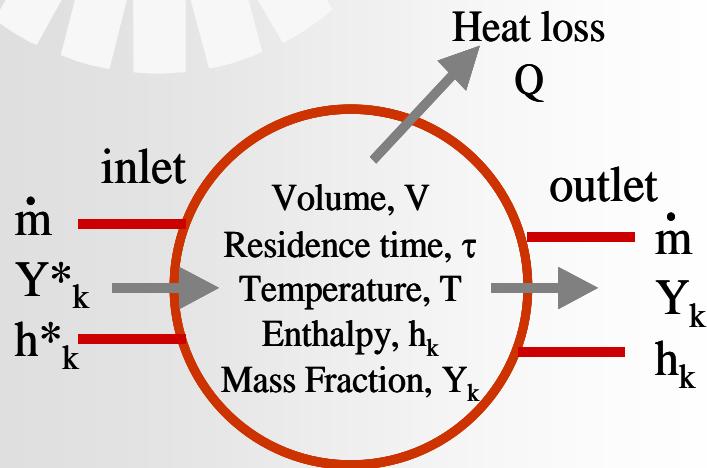
- LBO data for jet fuels and solvents



Modeling Methods – Physical Models

Simplified, kinetics-based model of physical problem (CHEMKIN based)

- Lean Blow Off – Extinction of a ‘Perfectly Stirred Reactor’



Surrogate Selection – preliminary (awaiting new data)

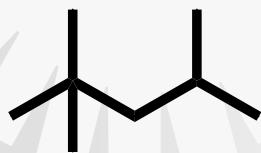
- Targets – Chemical classes, MW

Reaction model complied from JetSurf, SERDP, LLNL (iso-octane) + new isododecane model

	ONR - JP-5		ONR - JP-5 (HRJ)		ONR - JP-5 (HRJ) - a		Sasol IPK	
	Liq vol fraction	Mass fraction	Liq vol fraction	Mass fraction	Liq vol fraction	Mass fraction	Liq vol fraction	Mass fraction
n-decane		0		0		0		0
n-dodecane		0	35	0.358	35	0.349		0
n-tetradecane		0		0		0		0
n-cetane (n-hexadecane)	43	0.428	25	0.264	25	0.257		0
iso-octane (2,2,4-trimethylpentane)	20	0.178	40	0.378		0	20	0.188
2,2,4,6,6-pentamethylheptane		0		0	40	0.394	70	0.704
methylcyclohexane	15	0.149		0		0		0
n-butylcyclohexane		0		0		0	10	0.109
m-xylene (1,3)	22	0.245		0		0		0
	grams/cc	0.776	grams/cc	0.732	grams/cc	0.751	grams/cc	0.736
	MW	137.5	MW	152.1	MW	181.9	MW	152.7
	H/C	1.903	H/C	2.19	H/C	2.16	H/C	2.16
	BP(K)	462.8	BP(K)	463.8	BP(K)	493.3	BP(K)	438.1
	Shell GTL		Linpar 1416		L-142		L-210	
	Liq vol fraction	Mass fraction	Liq vol fraction	Mass fraction	Liq vol fraction	Mass fraction	Liq vol fraction	Mass fraction
n-decane	30	0.305116		0		0		0
n-dodecane		0	30	0.293		0	10	0.099
n-tetradecane		0		0		0		0
n-cetane (n-hexadecane)		0	70	0.707		0	5	0.051
iso-octane (2,2,4-trimethylpentane)	40	0.386		0		0		0
2,2,4,6,6-pentamethylheptane	30	0.309		0	30	0.286	60	0.589
methylcyclohexane		0		0	20	0.198		0
n-butylcyclohexane		0		0	50	0.515	15	0.159
m-xylene (1,3)		0		0		0		0
	grams/cc	0.718	grams/cc	0.766	grams/cc	0.775	grams/cc	0.753
	MW	136.3	MW	206.5	MW	135.6	MW	171.0
	H/C	2.21	H/C	2.14	H/C	2.05	H/C	2.13
	BP(K)	420.2	BP(K)	539.4	BP(K)	438.0	BP(K)	466.4

Iso-dodecane Combustion Model

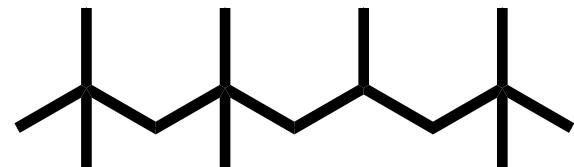
Higher MW iso-alkane oxidation model needed to match jet fuel MW



Iso-Octane
(2,2,4 tri-methyl-pentane)

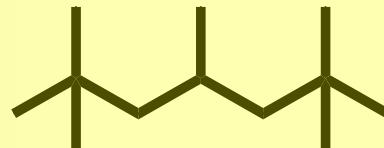
-Gasoline primary reference fuel

Detailed model unavailable



Iso-Cetane
(2,2,4,4,6,8,8 hepta-methyl-nonane)

-Diesel reference fuel

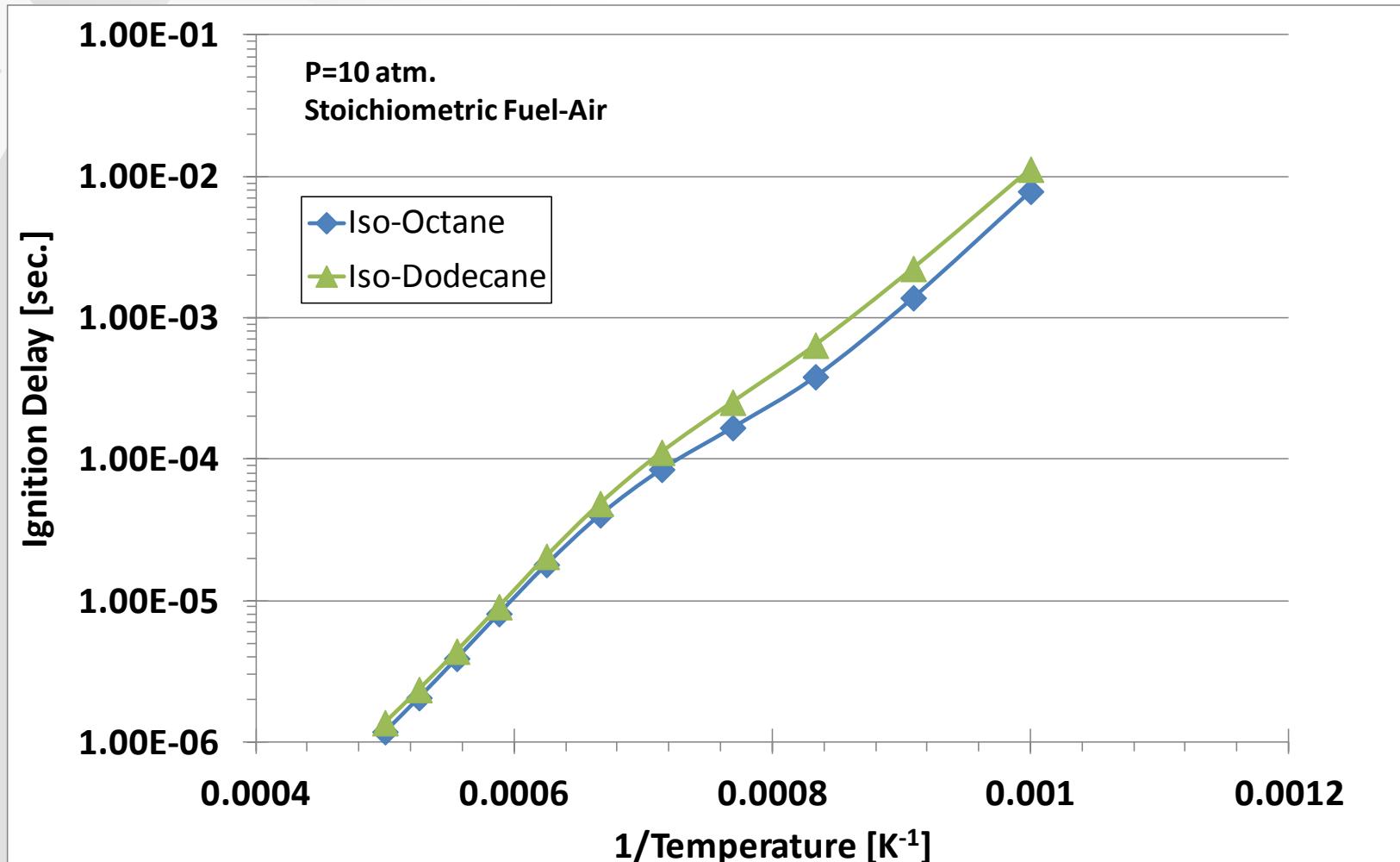


Iso-Dodecane
(2,2,4,6,6 penta-methyl-heptane)

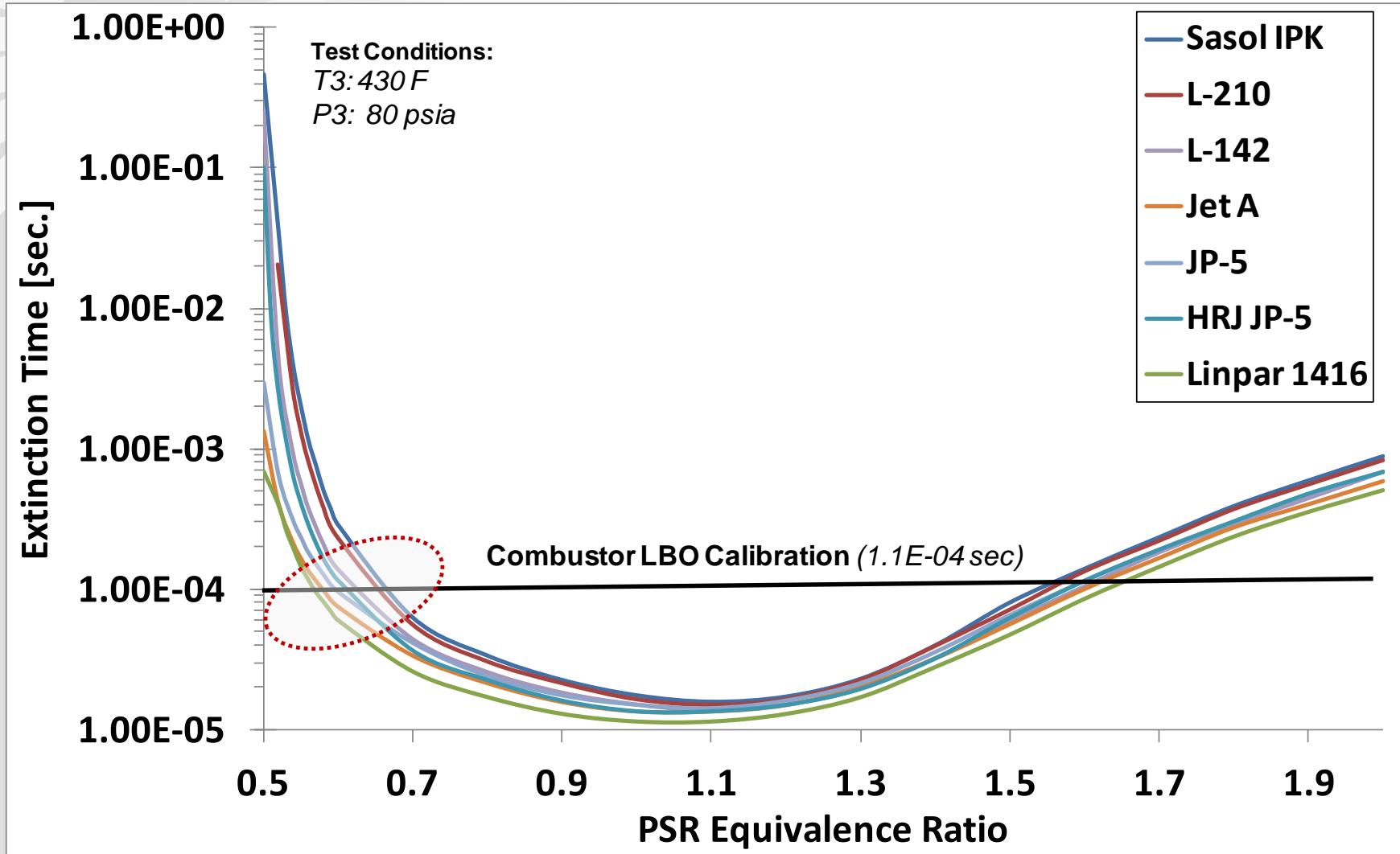
Constructed by analogy from Curran, et al iso-octane model
Pyrolysis portion validated against data (see Zeppieri, et al)

Oxidation Model Benchmarked Against Iso-Octane Model

*Iso-Dodecane ignition delay comparable to iso-octane value above ~1500 K;
Iso-C12 delay ~ 1.3-1.75 x Iso-C8 delay below 1500K*

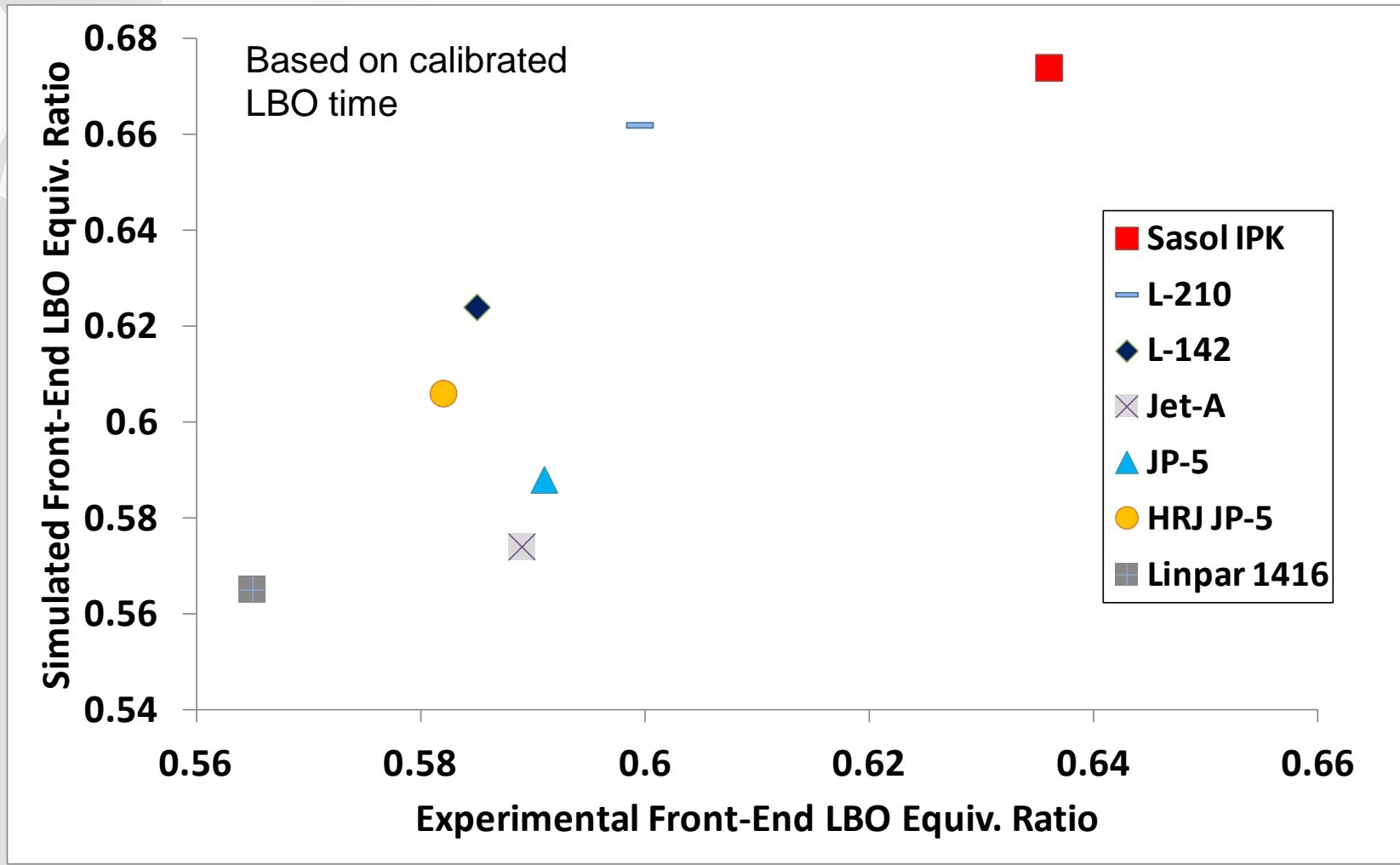


Computed Stirred Reactor Extinction Times



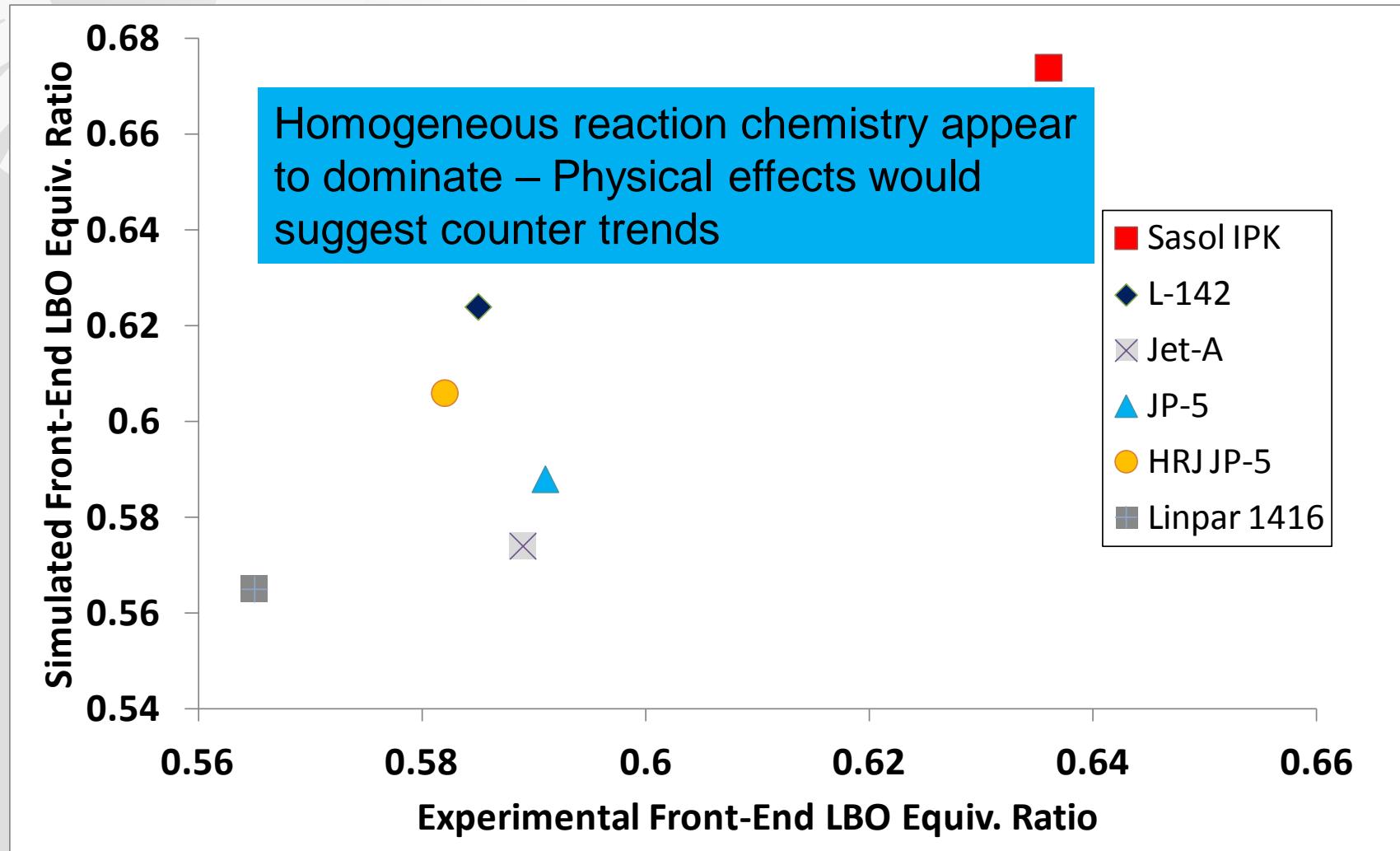
Comparison to Model Calculations

PSR Extinction Times consistent with Experimental Trends

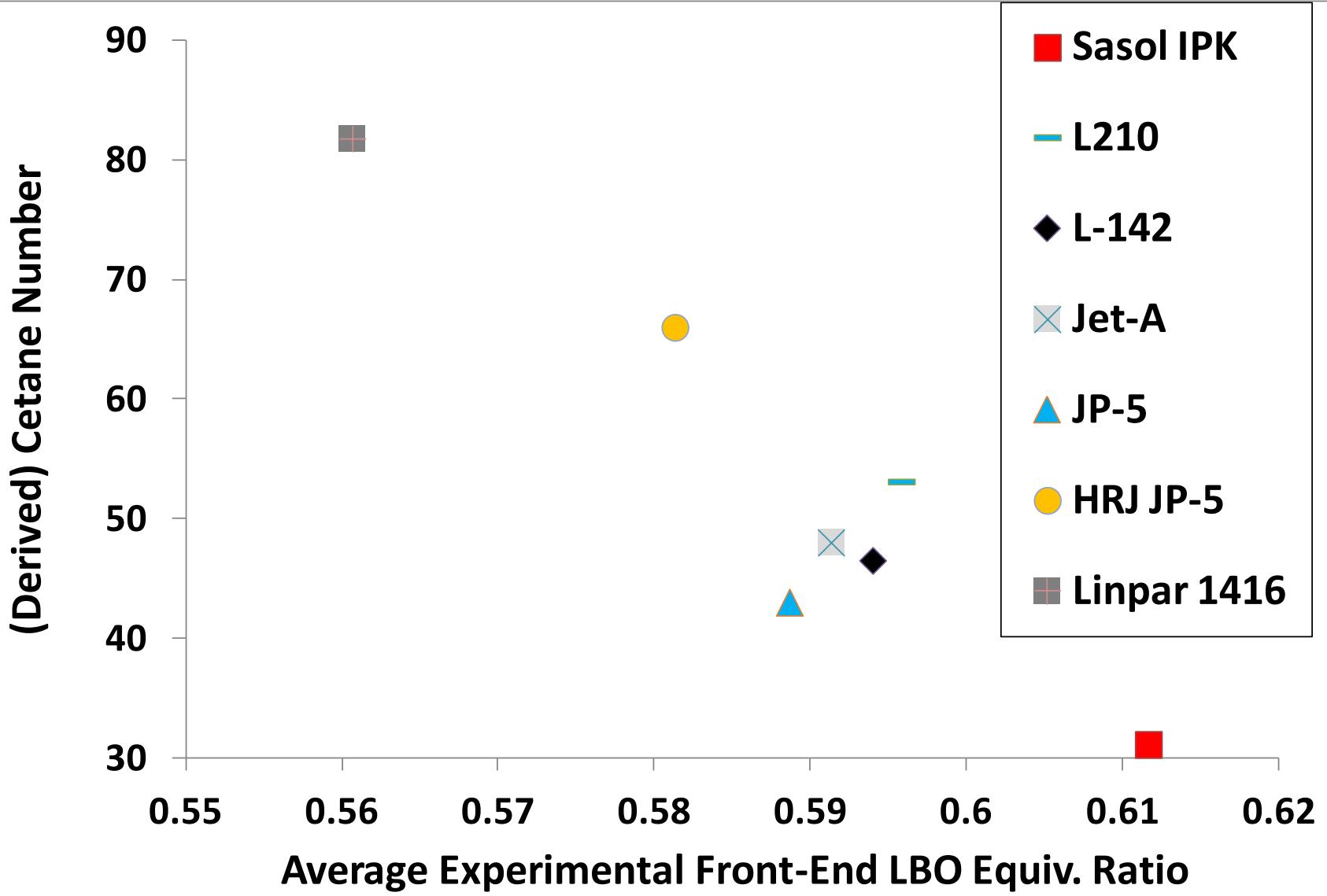


Comparison to Model Calculations

PSR Extinction Times consistent with Experimental Trends



Or ---- LBO Correlates with DCN even Better!



Objectives and Outline

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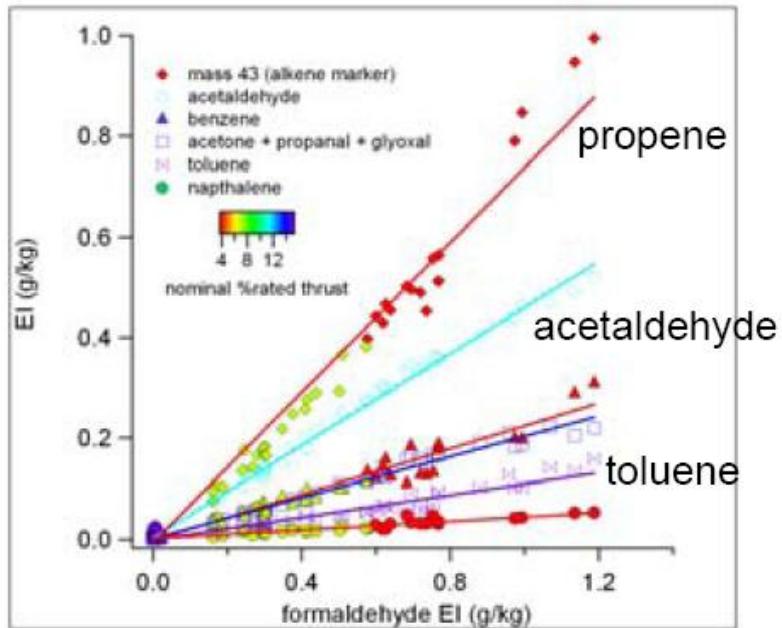
Outline:

- New data sets – performance of fuels in research combustor
 - Fuel selection
 - Combustor
 - Emissions, LBO data
 - Surrogates and Predictions
- **Hydrocarbon Emission Fingerprint** ←————
 - Discussion of controlling phenomena
 - Quantitative comparisons
- Brief update on AF Rules and Tools program
- Summary
- Recommendations

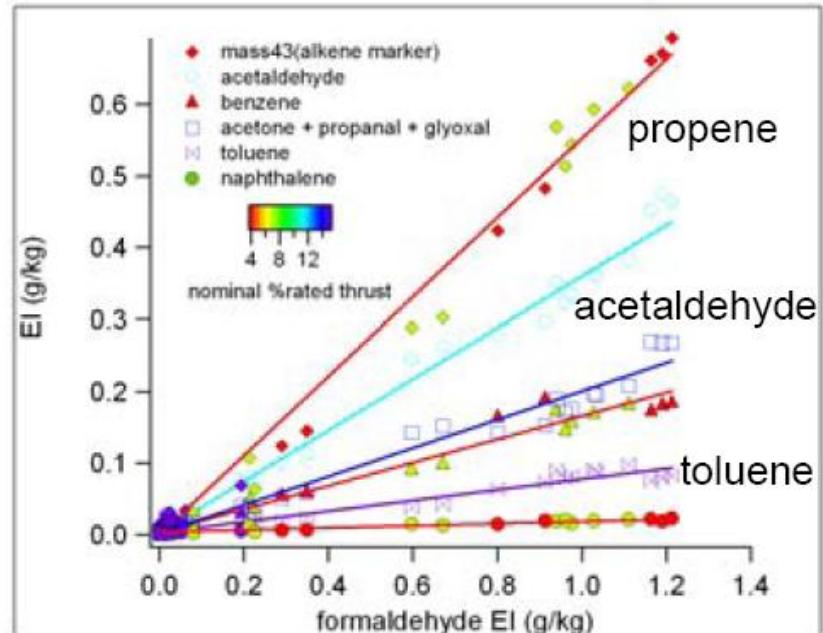
Challenge Problem: HC Emissions from Gas turbine Engines

Empirical evidence that emissions scale linearly – independent of engine or power

APEX 2



APEX 3



Includes 4 B737s.

Includes 1-B737, 2-B757, 1-A300.

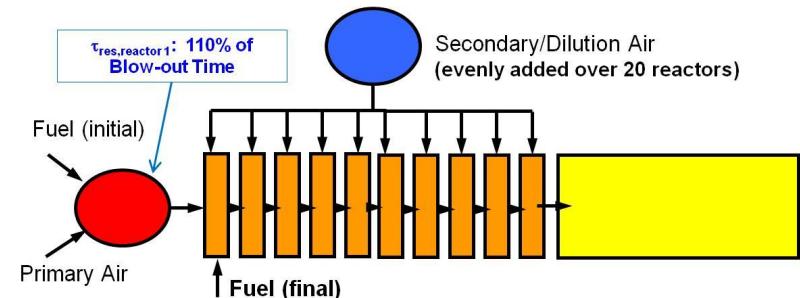
- What physical/chemical processes control this scaling?
- Can impact of alternative fuels on atmospheric pollution be anticipated?

Approach – presented last year

Identify chemistry and physics controlling scalability of HC emissions

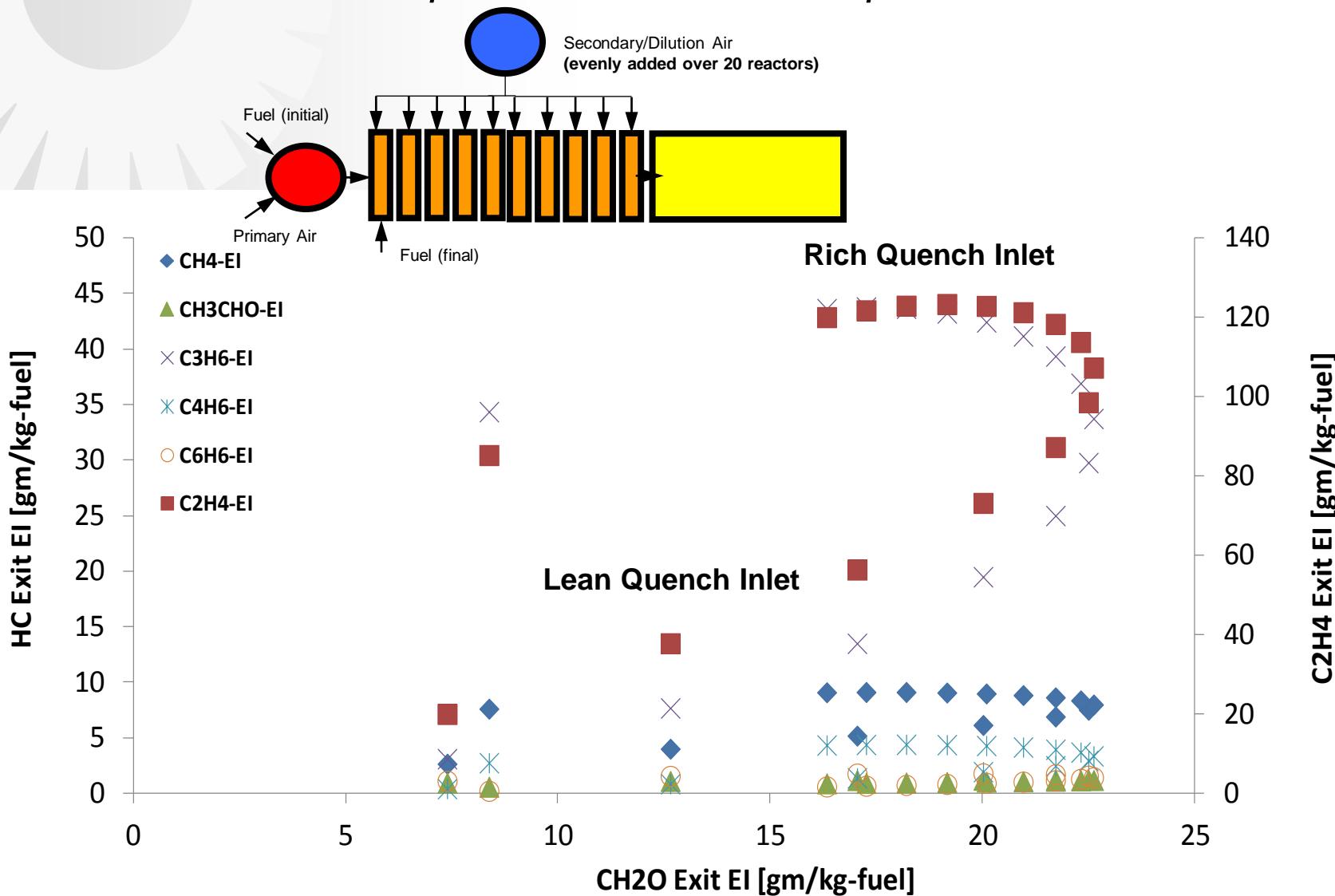
Methodology:

- Utilize reactor-network formulation to simulate flowfield of burner
- Fuel used: 77% dodecane, 23% m-xylene (vol %) – SERDP mechanism
- Initially assumed “bulk flow” conditions (e.g., total flow rates, total burner volume, etc.)
- Modified to focus on conditions with measurable emission levels and those exhibiting scaling
- Approximate “Idle”/low-power conditions:
 $P_3 = 4.08 \text{ atm}$,
 $T_3 = 478 \text{ K}$
 $\Phi \text{ overall } \sim 0.25$
-
- Good Results – but Reactor Model: **Too Complex!!!!**



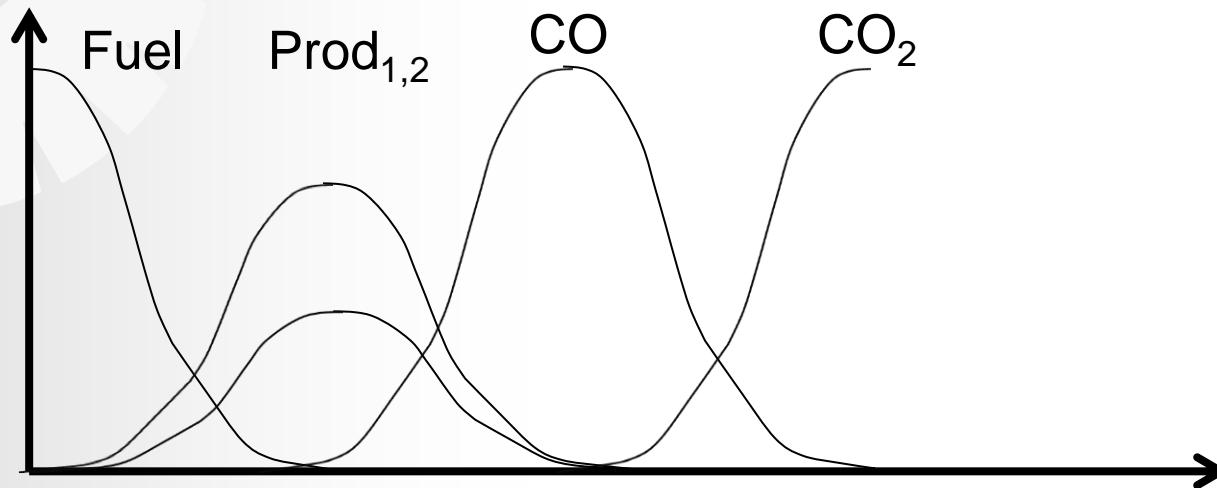
Reactor Network Solutions – Phi Sweep

UHC EI are functions of equivalence ratio of first quench reactor



Hypothesis for Fingerprint

Related to known oxidation sequence



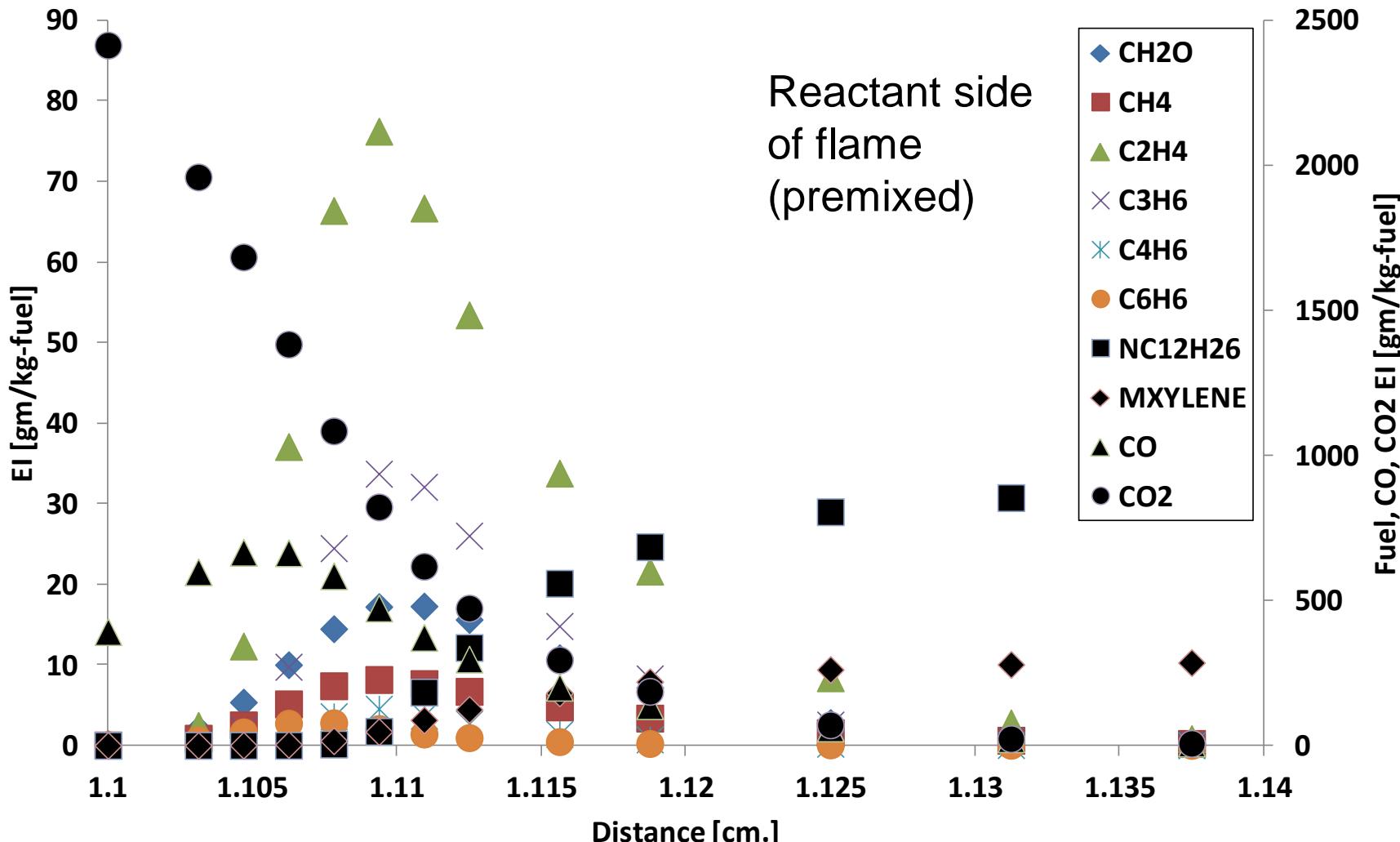
$\text{Prod}_1 \Leftrightarrow \text{Prod}_2$ (?) - or just decomposition species



$\text{Prod}_1, \text{Prod}_2$ stay in constant ratio – formation and decay

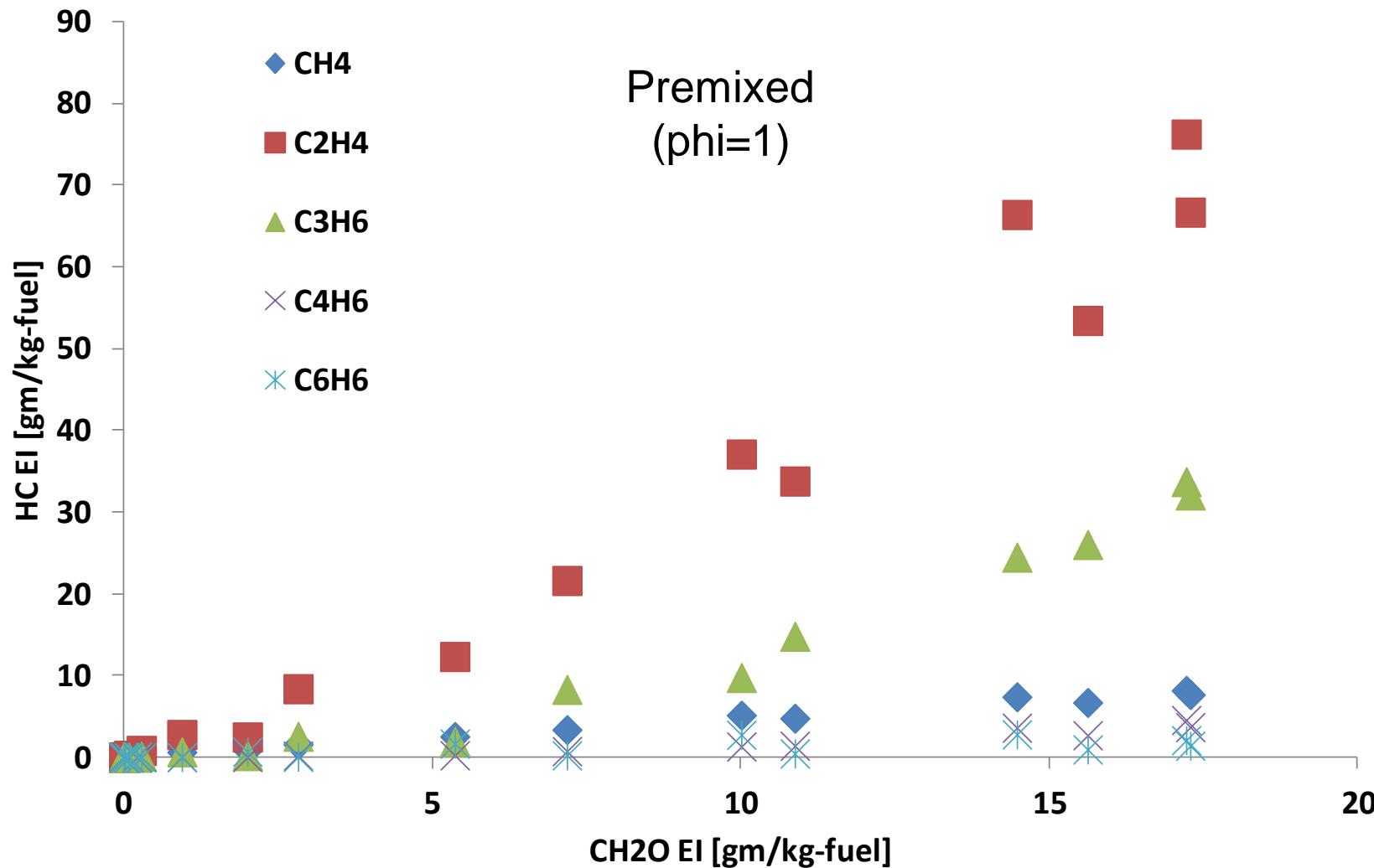
Example: Structure of Opposed Jet Flame (premixed)

Scaling of HC species corresponds to fuel chemistry (decomposition of parent fuel)



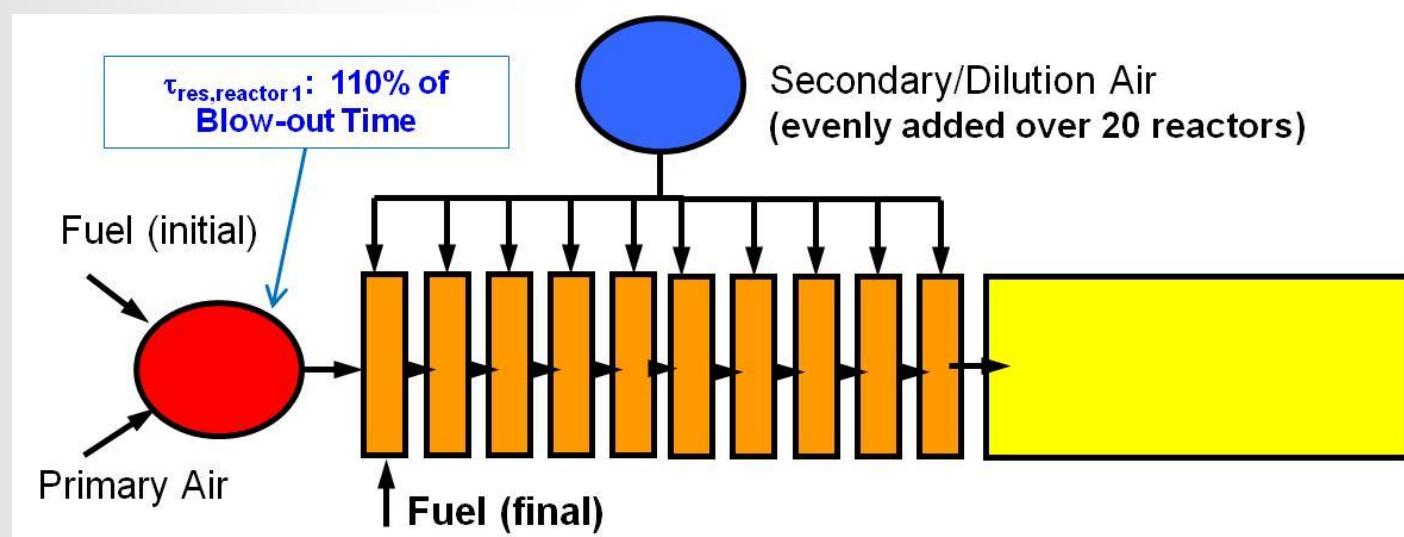
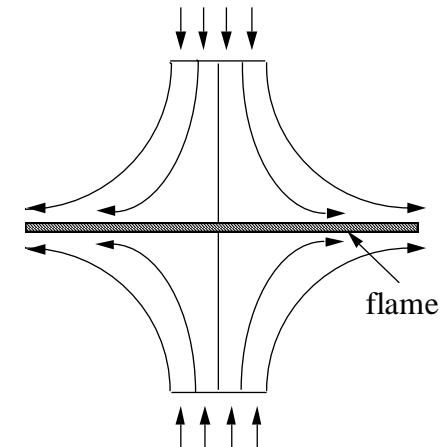
Example: Computed HC Ratios in Opposed Jet Flames

HC-EI Trends vs. CH₂O-EI very similar to trends from PSR Network Analysis



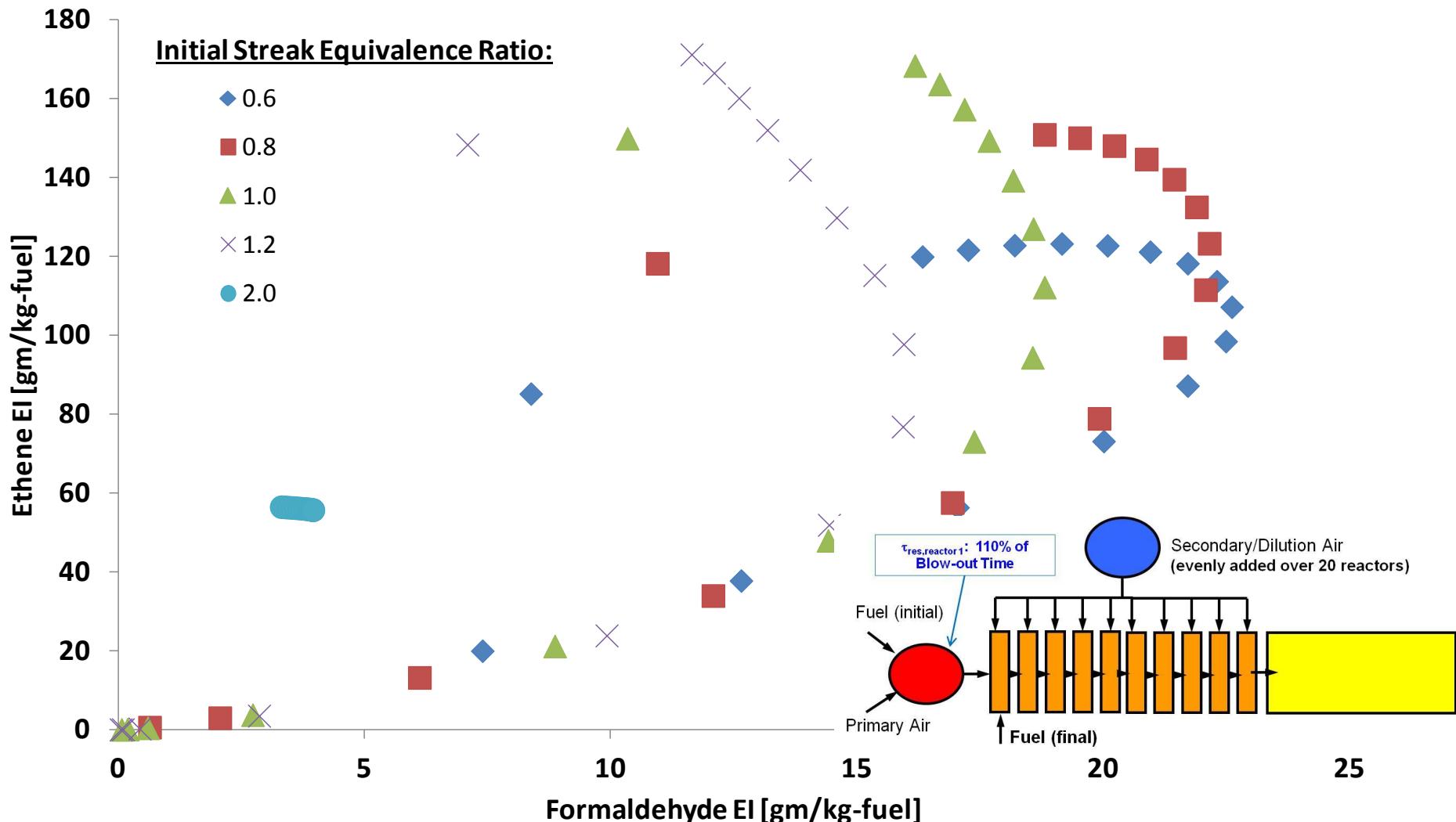
Extended studies

- Opposed jet – premixed (variable phi)
- Premixed flames (variable phi)
- Altered Network reactor assumptions
 - Variable initial equivalence ratio
 - Variable initial reactor residence time
 - Variable quench time



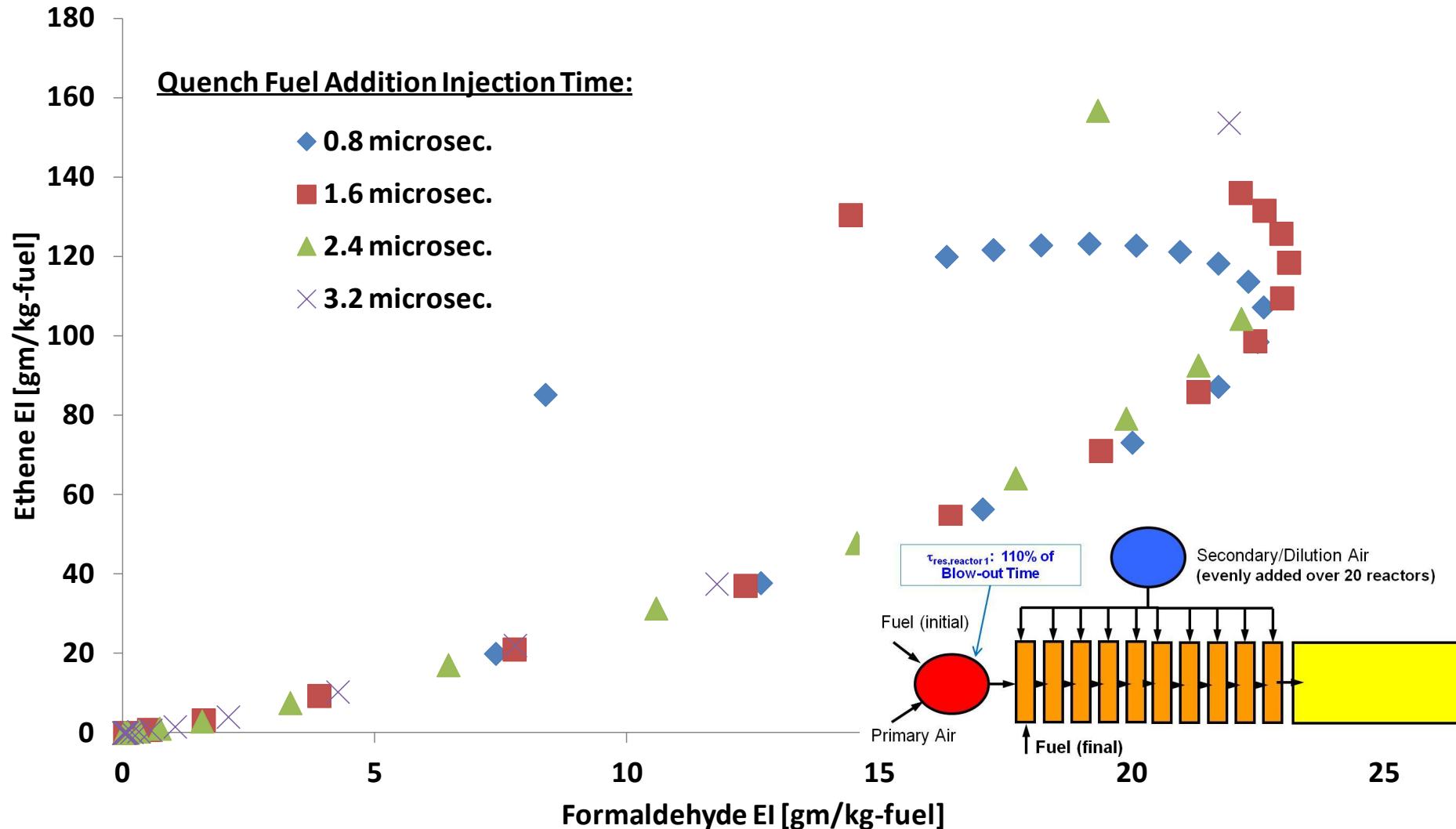
Example : Impact of Initial Equivalence Ratio

Lower branch shows scaling of EI values



Impact of Quench Time (in first quench reactor)

Scaling independent of injection time up to point of peak CH₂O formation



Computed Scaling Factors vs. Experiments

Similar results amongst model assumptions AND reasonable agreement with experimental data

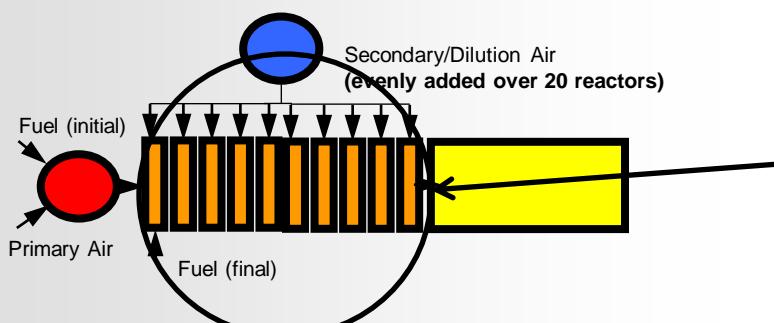
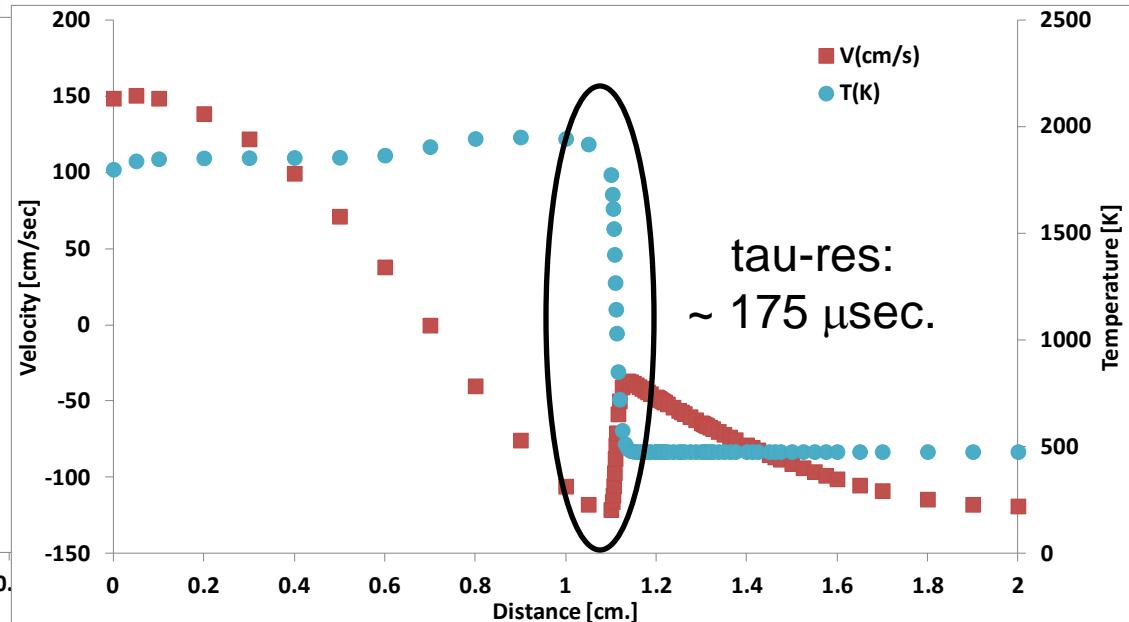
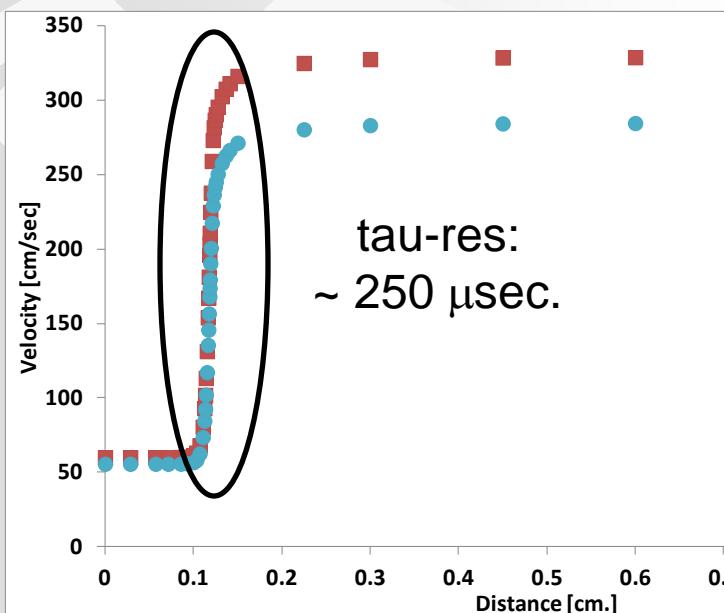
	Model Predictions					Engine Data	
	PSR Network	Opposed Jet	Opposed Jet	Pre-mixed	Pre-mixed	Spicer	Aerodyne
	(Lean Side)	(Burned (0.6) vs. Fuel/Air)	(Fuel/Air (1.0) vs. Fuel/Air)	Phi = 0.6	Phi = 1.0	(JP-5/CFM-56/idle)	(AAFEX/JP-8)
CH4	0.44	0.49	0.72	0.42	0.76	0.43	-
C2H4	3.27	4.25	3.93	3.2	4.2	2.69	1.33
C3H6	0.61	1.63	1.59	1.45	1.66	0.79	0.51
C4H6	0.06	0.23	0.14	0.14	0.15	0.3	-
C6H6	0.17	0.18	0.09	0.05	0.1	0.32	0.16

Lean side –
independent of
model
assumptions

- Scaling factors are slopes of HC-EI/CH2O-EI correlations
- All models used SERDP mechanism with n-Dodecane/m-Xylene Fuel

Time Scale Considerations

Quench time-scales need to be significantly **less than reactive** flame-front residence times



PSR-quench time scales: 20 $\mu\text{sec.}$

AF – Rules and Tools Program

- Restarted late last spring
- Combustor rig preliminary design complete
- Rig construction and testing not expected until mid next year
- Fuels selected (~10)
- Combustion tests recommended for the fuels
 - Extinction strain rate
 - Ignition
 - Flow reactor speciation

Conclusions – Emission and LBO tests

- Lean Blow-off limits trend with chemical nature of fuel
 - Pure n-alkane fuel is most robust
 - Largely branched i-alkanes least robust
 - Physical effects not quantified but appear to be minor
 - Correlates with PSR extinction and DCN
- Near to blow-off (not shown) CO emissions trend similarly
- Higher power CO emissions – no clear trend
- NOx emissions nearly identical
 - Small decrease with alkane fuels

Conclusions – Hydrocarbon Fingerprint

- Network PSR quench model yields linear relationship amongst selected hydrocarbon products
 - relatively independent of initial assumptions
- Linear relationships also observed through flame-fronts of opposed-jet and premixed fuel-air systems
- Calculated emission index ratios (HCEI/CH₂OEI) from PSR Network, opposed-jet and premixed flame calculations are qualitatively similar to each other and to experimental values
- Quenching must occur faster than progression of reaction front, e.g., 10-50 microseconds
- Preliminary results (not shown) indicate results dependent on surrogate chemistry

Recommendations - 2012

- Assess LBO – DCN correlation generality – or limitations
 - Plot of DCN vs. extinction for surrogate compounds?
 - Reactivity index
- Mechanisms – with defined accuracies/uncertainties – how to quantify?
- Robust surrogate generation method
- (Better) Validated mechanisms for monocyclic and bicyclic alkanes

Thank You!!!!

